wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 02:00 PM EDT

PDB ID	:	1JRQ
Title	:	X-ray Structure Analysis of the Role of the Conserved Tyrosine-369 in Active Site of E. coli Amine Oxidase
Authors	:	Murray, J.M.; Kurtis, C.R.; Tambarajah, W.; Saysell, C.G.; Wilmot, C.M.; Parsons, M.R.; Phillips, S.E.V.; Knowles, P.F.; McPherson, M.J.
Deposited on	:	2001-08-14
Resolution	:	2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

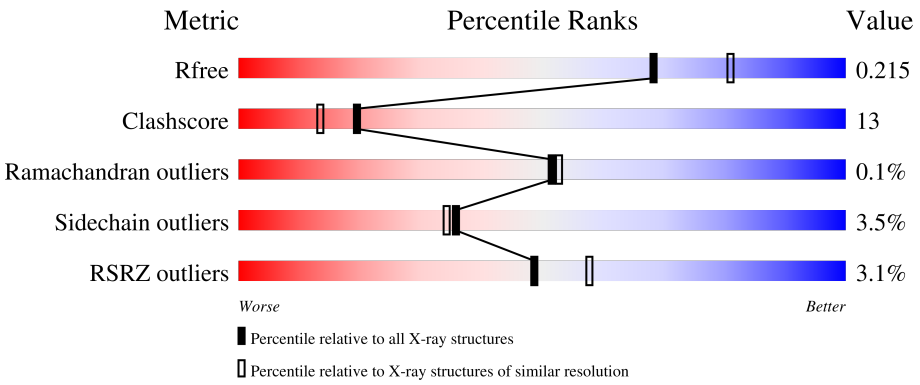
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	2% 71% 25% • •
1	B	727	4% 74% 22% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12750 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Copper amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	718	5663	3602	964	1075	22	0	0	0
1	B	721	5687	3617	970	1078	22	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	369	PHE	TYR	engineered mutation	UNP P46883
A	466	TPQ	TYR	modified residue	UNP P46883
B	369	PHE	TYR	engineered mutation	UNP P46883
B	466	TPQ	TYR	modified residue	UNP P46883

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	2	2	2	0	0
3	B	2	2	2	0	0

- Molecule 4 is water.

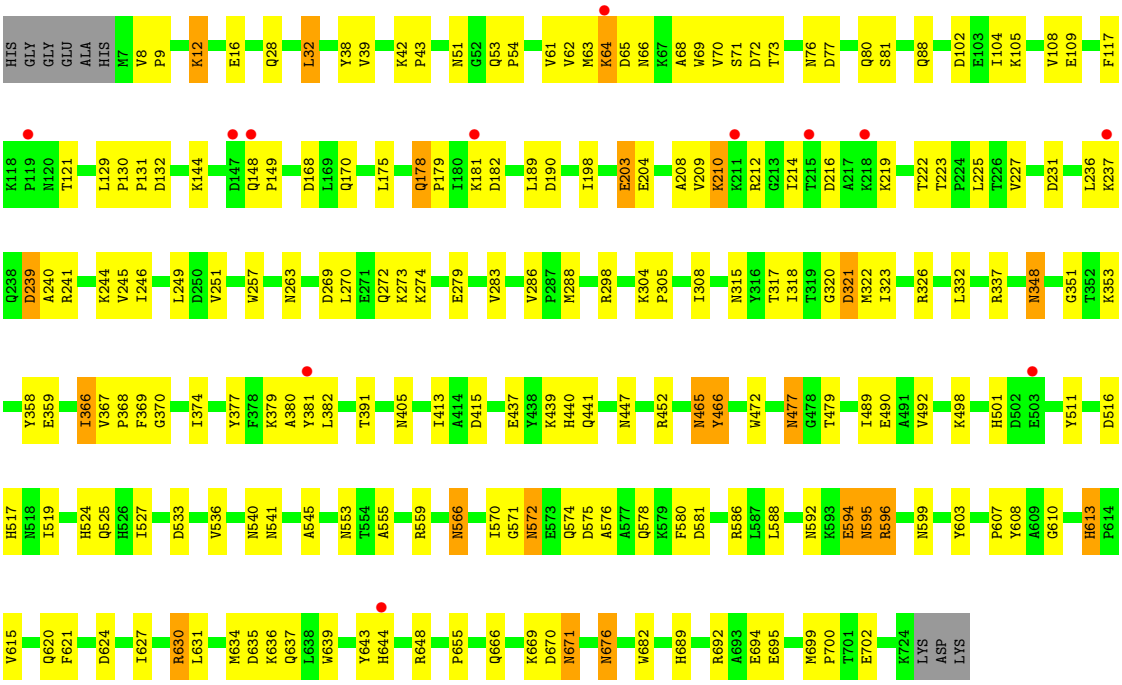
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	749	749	749	0	0
			Total	O		
4	B	645	645	645	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

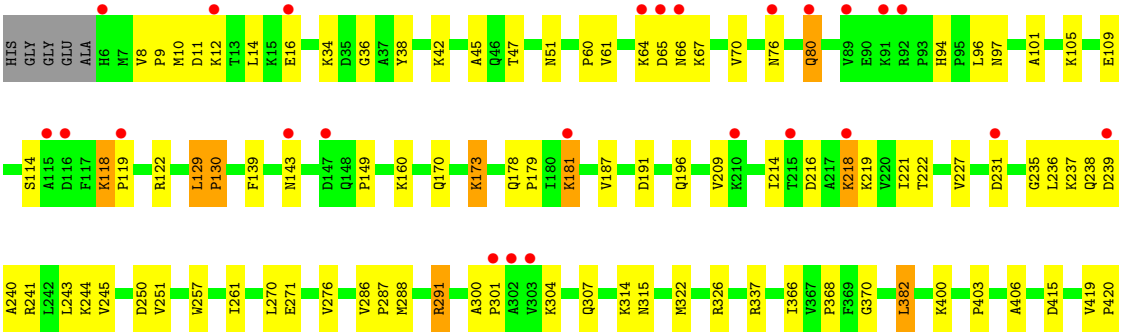
• Molecule 1: Copper amine oxidase

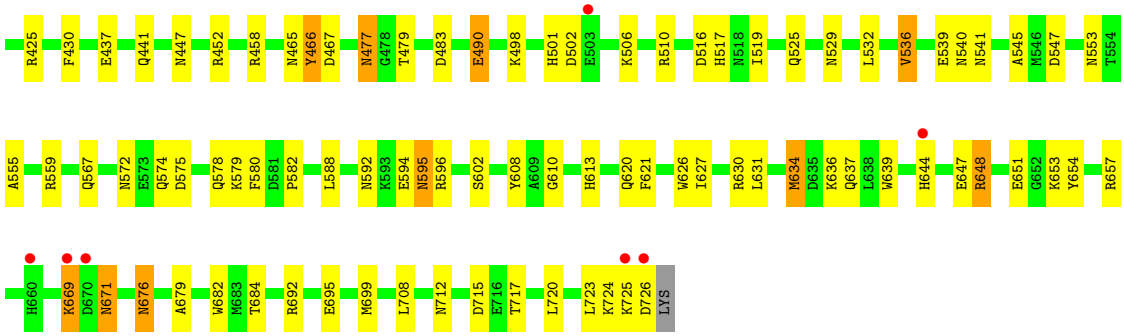
Chain A:



• Molecule 1: Copper amine oxidase

Chain B:




R425
F430
E437
Q441
N447
R452
R458
N465
Y466
D467
N477
G478
T479
D483
E490
K498
H501
D502
E503
K506
R510
D516
H517
N518
I519
Q525
N529
L532
V536
E539
N540
N541
A545
M546
D547
N553
T554
A555
R559
Q567
N572
E573
Q574
D575
Q578
K579
F580
D581
P582
L588
N592
K593
E594
N595
R596
S602
Y608
A609
G610
H613
Q620
F621
W626
I627
R630
L631
M634
D635
K636
Q637
L638
W639
H644
E647
R648
E651
G652
K653
Y654
R657
H660
K669
D670
N671
N676
A679
W682
M683
T684
R692
E695
M699
L708
N712
D715
E716
T717
L720
L723
K724
K725
D726
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	134.54Å 166.45Å 79.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 19.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-2.15) 92.6 (19.99-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.15Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.235 0.175 , 0.215	Depositor DCC
R_{free} test set	3092 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.785	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12750	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, CA, TPQ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.34	0/5792	1.24	32/7884 (0.4%)
1	B	0.33	0/5817	1.20	25/7917 (0.3%)
All	All	0.34	0/11609	1.22	57/15801 (0.4%)

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	692	ARG	NE-CZ-NH2	-15.20	112.70	120.30
1	A	326	ARG	NE-CZ-NH2	-13.58	113.51	120.30
1	A	692	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	A	596	ARG	CD-NE-CZ	9.35	136.69	123.60
1	B	291	ARG	NE-CZ-NH2	8.30	124.45	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5663	0	5539	158	0
1	B	5687	0	5562	146	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	749	0	0	16	0
4	B	645	0	0	20	0
All	All	12750	0	11101	288	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 288 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:ASN:HD22	1:B:671:ASN:HD21	1.07	0.99
1:A:225:LEU:HD22	1:A:381:TYR:HE2	1.28	0.96
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.48	0.95
1:A:304:LYS:H	1:B:315:ASN:HD21	1.13	0.91
1:B:322:MET:HG3	4:B:1156:HOH:O	1.73	0.89

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	715/727 (98%)	688 (96%)	27 (4%)	0	100 100
1	B	718/727 (99%)	693 (96%)	23 (3%)	2 (0%)	41 37
All	All	1433/1454 (99%)	1381 (96%)	50 (4%)	2 (0%)	51 53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	536	VAL
1	B	130	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	609/615 (99%)	585 (96%)	24 (4%)	32	30
1	B	611/615 (99%)	592 (97%)	19 (3%)	40	39
All	All	1220/1230 (99%)	1177 (96%)	43 (4%)	36	34

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	114	SER
1	B	539	GLU
1	B	118	LYS
1	B	181	LYS
1	B	613	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	660	HIS
1	B	613	HIS
1	B	196	GLN
1	B	599	ASN
1	B	676	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPQ	B	466	1	13,14,15	2.41	5 (38%)	15,19,21	3.62	6 (40%)
1	TPQ	A	466	1	13,14,15	2.24	4 (30%)	15,19,21	3.63	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	B	466	1	-	0/5/22/24	0/1/1/1
1	TPQ	A	466	1	-	2/5/22/24	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	TPQ	C1-C2	-5.08	1.41	1.49
1	A	466	TPQ	C1-C2	-4.98	1.41	1.49
1	B	466	TPQ	C6-C5	-4.22	1.33	1.44
1	A	466	TPQ	CB-C1	3.62	1.57	1.50
1	B	466	TPQ	CB-C1	3.28	1.57	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	466	TPQ	CB-CA-C	-12.05	88.88	111.47
1	B	466	TPQ	CB-CA-C	-11.39	90.11	111.47
1	A	466	TPQ	CA-CB-C1	-5.10	103.76	113.51
1	B	466	TPQ	CA-CB-C1	-5.09	103.79	113.51
1	B	466	TPQ	C6-C5-C4	3.23	122.51	117.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466	TPQ	C2-C1-CB-CA
1	A	466	TPQ	C6-C1-CB-CA

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	466	TPQ	4	0
1	A	466	TPQ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	717/727 (98%)	-0.35	12 (1%)	70	76	15, 26, 46, 62	0
1	B	720/727 (99%)	-0.23	32 (4%)	34	43	17, 29, 50, 65	0
All	All	1437/1454 (98%)	-0.29	44 (3%)	49	58	15, 28, 48, 65	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	HIS	7.6
1	B	726	ASP	5.4
1	B	115	ALA	5.1
1	B	91	LYS	4.4
1	A	64	LYS	4.4

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPQ	A	466	14/15	0.78	0.21	20,43,47,48	0
1	TPQ	B	466	14/15	0.87	0.18	22,45,49,50	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	B	803	1/1	0.92	0.09	54,54,54,54	0
3	CA	A	803	1/1	0.94	0.12	54,54,54,54	0
2	CU	A	801	1/1	0.99	0.07	28,28,28,28	0
3	CA	B	802	1/1	0.99	0.13	29,29,29,29	0
3	CA	A	802	1/1	0.99	0.12	26,26,26,26	0
2	CU	B	801	1/1	1.00	0.05	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.